

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.18×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.89×10^{-1}

Confidence level: 7.70×10^{-1}

Nearest Neighbors from the Training Set

[Image not found](#)

(3Z)-3-Hexenyl acetate

Measured: 7.80×10^{-11}

Predicted: 7.52×10^{-11}

[Image not found](#)

Dimethyl adipate

Measured: 8.40×10^{-12}

Predicted: 6.84×10^{-12}

[Image not found](#)

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80×10^{-11}

Predicted: 4.73×10^{-11}

[Image not found](#)

Dimethyl glutarate

Measured: 3.30×10^{-12}

Predicted: 3.76×10^{-12}

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Dimethyl succinate

Measured: 1.40×10^{-12}

Predicted: 1.93×10^{-12}